

**CRYSTALLOGRAPHY-RELATED METHOD FOR IDENTIFYING  
POTENTIAL INHIBITORS OF THE CD4-GP120 INTERACTION**

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**Abstract of the Disclosure**

10 The subject invention provides a crystal suitable for  
X-ray diffraction comprising a polypeptide having an  
amino acid sequence of a portion of a Human  
Immunodeficiency Virus Type I envelope glycoprotein  
gp120. The subject invention also provides the above-  
described crystals, wherein the crystal is arranged in  
15 a space group  $P222_1$ , so as to form a unit cell of  
dimensions  $a=71.6 \text{ \AA}$ ,  $b=88.1 \text{ \AA}$ ,  $c=196.7 \text{ \AA}$ , and which  
effectively diffracts x-rays for determination of the  
atomic coordinates of the gp120 to a resolution of  $2.5 \text{ \AA}$   
or better. The subject invention additionally  
20 provides compounds inhibiting the human CD4-gp120  
interaction, compounds inhibiting chemokine receptor-  
gp120 interaction, mimics of human CD4, gp120 variants  
and uses thereof.